Towards quantitative resolution analysis of 3-D EM inversion results. Efficient calculation of the Hessian matrix of frequency-domain EM data misfit using adjoint sources approach

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SUMMARY

We discuss in this abstract an efficient computation of the Hessian matrix of EM data misfit based on adjoint sources approach. We consider this work as a step to the development of quantitative resolution schemes in electromagnetic (EM) frequency-domain problems based on analysis of an inverse of the Hessian matrix. In addition to being the carrier of resolution information the Hessian can be interpreted as an inverse of a posterior model covariance matrix. This interpretation provides a way for better regularization of the inverse problem. We state that using adjoint sources approach one can calculate the Hessian matrix for a price of $O(N)$ forward problem calls per frequency and polarization, where N stands for dimension of model parameter space. Thus this approach allows for substantial computational savings during Hessian computation compared to brute-force approach (numerical differentiation) which requires $O(N^2)$ forward problem calls per frequency and polarization. Moreover adjoint sources approach allows for $exact$ estimation of the elements of Hessian matrix, which is not the case if $approximate$ brute-force numerical differentiation is invoked.

Keywords: 3-D EM inversion, resolution analysis, Hessian matrix, regularization, adjoint sources approach

INTRODUCTION

A number of rigorous three-dimensional (3-D) frequency-domain electromagnetic (EM) inverse solutions have been developed in the past two decades both in Cartesian (e.g. Mackie and Madden, 1993, Newman and Alumbaugh, 2000, Haber, Asher, and Oldenburg, 2004, Siripunvaraporn, Egbert, Lenbury, and Uyeshima, 2005, Sasaki and Meju, 2006, Avdeev and Avdeeva, 2009, Egbert and Kelbert, 2012, Zhang, Koyama, Utada, Yu, and Wang, 2012) and spherical geometries (e.g. Koyama, 2001, Kelbert, Egbert, and Schultz, 2008, Kuvshinov and Semenov, 2012, Koch and Kuvshinov, 2013, Püthe and Kuvshinov, 2013). Despite a certain success of 3-D EM analysis of frequency-domain data of different type and origin (e.g. Hautot et al., 2000, Newman, Recher, Tezkan, and Neubauer, 2003, Kelbert, Schultz, and Egbert, 2009, Utada, Koyama, Obayashi, and Fukao, 2009, Patro and Egbert, 2011, Semenov and Kuvshinov, 2012) the quantification of the model resolution is generally deficient. Till now the resolution studies are mostly based (if applied at all) on synthetic inversions for checkerboard input structures or/and on the visual inspection of the obtained images. At least two factors complicate the resolution analysis in 3-D EM inversion. First, the data depend very non-linearly on the conductivity distribution, thus making well-elaborated techniques of linear inverse theory (e.g. Tarantola, 2005) not applicable. Second, the dimension of the model space and computational expenses of 3-D forward problem solutions prohibit the application of probabilistic approaches (e.g. Mosegaard and Tarantola, 1995, Tompkins, Martinez, Alumbaugh, and Mukerji, 2011) that in principle may account for non-linearity using Monte-Carlo sampling.

WHY HESSIAN?

It is known that one can gain ample information about the inverse solution from the quadratic approximation of the penalty functional in the vicinity of the minimum. To illustrate the concept let us assume that vector $\mathbf{m} = (\sigma_1, \sigma_2, ..., \sigma_N)^T$ defines the model parametrization, where superscript T stands for transpose and $\sigma_1, \sigma_2, ..., \sigma_N$ are conductivities in N cells of the volume where we aim to recover conductivity distribution. By formulating inverse problem (conductivity recovery) as a minimization problem with a penalty function in a form of misfit β_d one can state that the solution $\mathbf{m}_0$ of minimization problem is a stationary point of β_d, i.e. $\mathbf{m}_0$ satisfies the following equation

$$\left.\frac{\partial \beta_d}{\partial \mathbf{m}}\right|_{\mathbf{m}_0} = 0. \quad (1)$$

This, in particular, means that the local behaviour of the misfit function $\beta_d(\mathbf{m})$ in a vicinity of a stationary point $\mathbf{m}_0$ is determined by the second-order terms of Taylor series

$$\beta_d(\mathbf{m}) \approx \beta_d(\mathbf{m}_0) + \frac{1}{2}\Delta\mathbf{m}^T \mathbb{H}(\mathbf{m}_0)\Delta\mathbf{m}, \quad (2)$$

where $\Delta\mathbf{m} = \mathbf{m} - \mathbf{m}_0$, $\mathbb{H}$ is the Hessian matrix, which in our example problem setup has a form

$$\mathbb{H}(\mathbf{m}_0) = \left.\begin{pmatrix} \frac{\partial^2\beta_d}{\partial\sigma_1\partial\sigma_1} & \frac{\partial^2\beta_d}{\partial\sigma_1\partial\sigma_2} & \cdots & \frac{\partial^2\beta_d}{\partial\sigma_1\partial\sigma_N} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial^2\beta_d}{\partial\sigma_N\partial\sigma_1} & \frac{\partial^2\beta_d}{\partial\sigma_N\partial\sigma_2} & \cdots & \frac{\partial^2\beta_d}{\partial\sigma_N\partial\sigma_N} \end{pmatrix}\right|_{\mathbf{m}_0}. \quad (3)$$

Analysis of eq. (2) suggests a way (Pankratov and Kuvshinov, 2013) to specify the bounds within which the optimal model $\mathbf{m}_0$ can be perturbed without increasing $\beta_d(\mathbf{m}_0)$ beyond a predefined value $\beta_d(\mathbf{m}_0) + \Delta\beta_d$, where $\Delta\beta_d$ is usually related to the noise in the data. In ultimate case when model parameters are independent, the Hessian matrix $\mathbb{H}$ and thus its inverse $\mathbb{H}^{-1}$ are diagonal matrices, leading to the following formula for perturbation $\Delta\mathbf{m}$ which does not increase misfit beyond $\Delta\beta_d$

$$\Delta m_l \equiv \Delta\sigma_l = \pm\sqrt{2\Delta\beta_d}\sqrt{\mathbb{H}_{ll}^{-1}}, \quad l = 1, 2, ...N, \quad (4)$$

with

$$\mathbb{H}_{ll}^{-1} = \frac{1}{\mathbb{H}_{ll}} = \left[\frac{\partial^2\beta_d}{\partial\sigma_l\partial\sigma_l}\right]^{-1}. \quad (5)$$

It is seen from eq. (4) that the larger values $\mathbb{H}_{ll}^{-1}$ correspond to larger admissible perturbations of m_l which do not influence β_d within threshold value $\Delta\beta_d$, meaning that m_l is poorly constrained (resolved); see also Figure 1 which illustrates the concept. However it is important to note here that usually model parameters are not independent thus making $\mathbb{H}$ and $\mathbb{H}^{-1}$ full-size matrices. This complicates resolution analysis since in this case there is no direct relation between admissible perturbation of specific m_l and specific element of $\mathbb{H}^{-1}$. Now, instead of eq. (4) more sophisticated formula holds (Pankratov and Kuvshinov, 2013) which nevertheless is also based on the inverse of Hessian matrix, $\mathbb{H}^{-1}$.

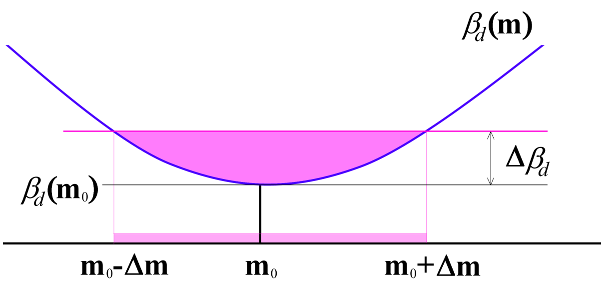

Figure 1. Illustrating equation (4).

In addition to being the carrier of resolution information the quadratic approximation (2) suggests the interpretation of $\mathbb{H}$ as an inverse posterior model covariance matrix. This interpretation provides an avenue for better regularization of the inverse problem. The idea behind this is based on the following argument. Usually regularization is performed by adding to a misfit a regularization term in a form

$$\beta_s = \lambda(\mathbf{m} - \mathbf{m}_p)^T D^T D(\mathbf{m} - \mathbf{m}_p), \quad (6)$$

and by searching during inversion – along with conductivity distribution – an appropriate regularization parameter, λ, which controls the smoothness of the model. Here D is a discrete representation of a gradient or higher order derivative operator, and $\mathbf{m}_p$ is the prior model. The conventional approach to determine optimal value of λ is based on L-curve technique. However our experience (and also experience of many others) shows that with real data this technique often does not work satisfactorily revealing unrealistic variations of conductivity both in vertical and lateral directions in the regions with poor spatial coverage by the data. The major reason for such behaviour is the lack of resolution for a priori unknown part of model parameters involved in the inversion. Incorporation of $\mathbb{H}$ into a regularization term

$$\beta_s = \lambda(\mathbf{m} - \mathbf{m}_p)^T \mathbb{H}(\mathbf{m} - \mathbf{m}_p), \quad (7)$$

helps, at least partially, to suppress undesirable impact of poorly resolved model parameters. Constructively one can first run inversion by minimizing the misfit term only, and then rerun inversion by implementing the regularization in the form of eq. (7) with $\mathbb{H}$ calculated at optimal point $\mathbf{m}_0$ during the first run.

Summing up we can state that $\mathbb{H}$ and $\mathbb{H}^{-1}$ indeed provides very useful diagnostic information for resolution analysis and, in addition, can be used for more appropriate regularization of the problem. However the question arises: what are the computational loads to calculate $\mathbb{H}$ and $\mathbb{H}^{-1}$? Calculation of $\mathbb{H}^{-1}$ can be naturally separated into two steps: 1) calculation of $\mathbb{H}$, and 2) calculation of an inverse of $\mathbb{H}$. Number of operations to calculate the inverse of $\mathbb{H}$ (second step) is proportional to N^α (cf. Press, Teulkovsky, Vetterling, and Flannery, 2007), where $2 < \alpha \leq 3$. As for $\mathbb{H}$ calculation, a straightforward option is brute-force approach based on numerical differentiation. In this case the number of operations to calculate $\mathbb{H}$ is $N^2 N_\Omega N_P K$, where N_Ω is a number of frequencies, N_P is a number of polarizations, and K is a number of operations to solve forward problem for a fixed frequency and polarization. It is evident that the first step is much more computationally expensive compared with the second step, since even for the most advanced 3-D EM frequency-domain forward problem solvers, $K = LN_f$, where N_f is a number of cells describing the forward problem modelling volume and L is a prefactor which varies with the solver but in any case significantly exceeds 1. Moreover in the most 3-D EM inversions number of searching parameters, N, is usually taken smaller or much smaller than N_f, $N < N_f$ making the difference between computational loads to calculate $\mathbb{H}$ and the inverse of $\mathbb{H}$ even higher. Bearing this in mind one can conclude that calculation of $\mathbb{H}$ is extremely computationally expensive if brute force approach is implemented. This motivated us to elaborate an approach which allows for calculation of the Hessian matrix, $\mathbb{H}$, as fast as possible.

We assert that the Hessian matrix – using adjoint sources approach – can be calculated for the price of $O(N)$ forward problem calls per frequency and polarization which is N times less compared with $\mathbb{H}$ computation based on brute-force approach. Since N in 3-D EM inversions of practical interest is usually large the adjoint approach allows for tremendous computational savings during $\mathbb{H}$ computation, thus making this task tractable.

NUMBER OF FORWARD PROBLEM CALLS FOR HESSIAN CALCULATIONS

By using a non-trivial mathematical machinery one can deduce that total number of forward problem calls which are needed to calculate Hessian matrix, $\mathbb{H}$, is

$$M_{AS} = N_P N_\Omega ((2 + N_P)N + N_S N_R + 2), \quad (8)$$

where N_P is a number of polarizations, N_Ω is a number of frequencies, N_S is a number of observation sites, and N_R is a number of different responses. All the details which lead to this result are presented in (Pankratov and Kuvshinov, 2013).

In magnetotellurics (MT) $N_P = 2$, and if we invert full MT tensor, i.e. $N_R = 4$, then the total number of forward problem calls to calculate $\mathbb{H}$ is

$$M_{AS,MT} = 4N_\Omega(2N + 2N_S + 1). \quad (9)$$

Another example is from controlled source (CS) electromagnetics – when receiver and transmitter are vertical magnetic dipoles (VMD). In this case $N_P = N_R = 1$, and thus the total number of forward problem calls to calculate $\mathbb{H}$ is:

$$M_{AS,VMD} = N_\Omega(3N + N_S + 2). \quad (10)$$

The latter estimate is also valid for 3-D global induction studies, if the source is described by first zonal harmonic and scalar C-responses are analyzed (i.e., again, $N_P = N_R = 1$).

By analyzing eq. (8) and taking in mind that in the most cases $N_S \leq N$ we immediately obtain that

$$M_{AS} = O(N), \quad (11)$$

per frequency and polarization. Note, again, that total number of forward problem calls which are needed to calculate Hessian matrix using brute-force approach is

$$M_{BF} = O(N^2), \quad (12)$$

per frequency and polarization.

CONCLUSIONS

We argue in this work that *exact* calculation of Hessian matrix, $\mathbb{H}$, becomes tractable if adjoint sources approach is implemented. We provide an estimate of a number of forward problem calls needed to calculate $\mathbb{H}$ using adjoint sources, which is N times less compared with *approximate* $\mathbb{H}$ computation based on brute-force approach. This estimate is obtained in an assumption that conductivity distribution is described by an isotropic (scalar) real-valued function. The extension to anisotropic (second-order tensor) and complex-valued conductivities is a topic of forthcoming study.

This work is intended to serve as a prelude to the development of quantitative resolution schemes in EM frequency-domain problems (both with natural and controlled sources) based on analysis of inverse of Hessian. In addition to being the carrier of resolution information the Hessian can be interpreted as an inverse posterior model covariance matrix. This interpretation provides an avenue for better regularization of the inverse problem.

One can argue that $O(N)$ forward problem calls per frequency and polarization is still a substantial computational burden to perform calculation of $\mathbb{H}$ (and subsequently $\mathbb{H}^{-1}$) routinely. But we aim to calculate $\mathbb{H}$ and $\mathbb{H}^{-1}$ only once (or very limited times), since our intention is not to implement them in Newton-like optimization schemes (during 3-D inversion), but to use it either for resolution analysis at a final step of 3-D inversion, or for better regularization of the problem.

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